

Application No. 09/359,181  
Docket No. 1028-1

Art Unit 1631  
Examiner: CLOW, LORI A.

In response to the Office Action dated May 21, 2002, please amend the above-identified application as follows:

IN THE CLAIMS:

Please amend the claims to read as follows:

1. <sup>(Thrice Amended)</sup> A computer-aided method for the provision, identification and description of molecules exhibiting a desired activity comprising:
  - a molecular modeling step in which molecular descriptors are determined computationally;
  - a step of building a combinatorial library of molecules;
  - a step of selecting candidate molecules which potentially exhibit said desired activity;
  - a filtering step whereby candidate molecules are filtered using at least one static filter representing a plurality of said molecular descriptors;
  - a further filtering step whereby candidate molecules are filtered using at least one dynamic filter representing constraints of conformational variations which each candidate molecule must satisfy in order to exhibit said desired activity.
10. <sup>(Thrice Amended)</sup> A computer-aided method according to Claim 9 wherein the static criteria are based on physiochemical and topological descriptors at least some of which are chosen from the following descriptors: Molar Mass; Ellipsoidal Volume; Molecular Volume; Molar Refractivity; Lipophilia (LogP); Kappa 1; Kappa 2; Kappa 3; Kappa Alpha 1; Kappa Alpha 2; Kappa Alpha 3; Flexibility; Kier Chi V4; Randic Index; Balaban Index; Weiner Index; Sum of Condition E; Dipolar Moment; Number of C Atoms; Number of O Atoms; Number of N Atoms; Number of H Atoms; Total Number of

Atoms; Number of Methyl Groups; Number of Ethyl Groups; Number of Amino Groups; Number of Hydroxyl Groups.

18. <sup>(Thrice Amended)</sup> A computer-aided method for the provision, identification and description of molecules exhibiting immunomodulatory activity comprising;

a step of molecular modeling in which molecular descriptors of a molecule having immunomodulatory activity are determined computationally;

a step of building a combinatorial library including molecules having said immunomodulatory activity;

a step of selecting candidate molecules which are potentially immunomodulatory;

a filtering step whereby candidate molecules are filtered using at least one static filter representing a plurality of said molecular descriptors; and

a further filtering step whereby candidate molecules are filtered using at least one dynamic filter representing constraints of conformational variations which each candidate molecule must satisfy in order to exhibit said immunomodulatory activity.

Please add the following claim:

73. A computer-aided method according to Claim 5 wherein the static criteria are based on physiochemical and topological descriptors at least some of which are chosen from the following descriptors: Molar Mass; Ellipsoidal Volume; Molecular Volume; Molar Refractivity; Lipophilia (LogP); Kappa 1; Kappa 2; Kappa 3; Kappa Alpha 1; Kappa Alpha 2; Kappa Alpha 3; Flexibility; Kier Chi V4; Randic Index; Balaban Index; Weiner Index; Sum of Condition E; Dipolar Moment; Number of C Atoms; Number of O Atoms; Number of N Atoms; Number of H Atoms; Total Number of Atoms; Number of Methyl Groups; Number of Ethyl Groups; Number of Amino